- (1) Propane; C_3H_8 ; [74-98-6]
- (2) Water; H₂O; [7732-18-5],
 at high pressure

EVALUATOR:

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December 1983

CRITICAL EVALUATION:

There have been five studies of this system at high pressures. The extensive study of De Loos $et\ al$. (1) was mainly concerned with the phenomenon of gas-gas immiscibility and although it is thought to be reliable the data are not strictly gas solubility. The data of De Loos $et\ al$. (1) are broadly consistent with data for other hydrocarbons + water mixtures. Sanchez and Coll (2) determined the phase behavior of this system in the region 200-400 °C and 20-300 MPa. Their data are not strictly gas solubility and are not in agreement with those of De Loos $et\ al$. (1).

The limited data of Wehe and McKetta (3) at 160 °F (344.3 K) are in excellent agreement with the smoothed values these workers obtained using the experimental data of Kobayashi and Katz (4). The data of Azarnoosh and McKetta (5) are also in reasonable agreement with the data of Wehe and McKetta (3). Of these three latter sets of data those of Azarnoosh and McKetta (5) are by far the most extensive and are classified as tentative. The degree of overlap of the three sets of data is too limited to enable a set of data to be recommended.

References

- De Loos, Th. W.; Wijen, A. J. M.; Diepen, G. A. M.
 J. Chem. Thermodyn. 1980, 12, 193.
- Sanchez, M.; Coll, R.
 An. Quim. 1978, 74, 132.
- Wehe, A. H.; McKetta, J. J.
 Anal. Chem. 1961, 33, 291.
- Kobayashi, R.; Katz, D. L.
 Ind. Eng. Chem. 1953, 45, 440.
- Azarnoosh, A.; McKetta, J. J.
 Pet. Ref. 1958, 37, 275.

- (1) Propane; C₃H₈; [74-98-6]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Azarnoosh, A.; McKetta, J.J.

Pet. Ref. 1958, 37, 275-278.

VARIABLES:

T/K: 288.7-410.9

P/kPa: 99-3409

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t1/°F	T ² /K	Total Pressure ¹ /psia	Partial Pressure ² P ₁ /kPa	Mol Fraction ¹ /10 ⁵ x ₁
60	288.7	(0.256) ³		
		(14.952) 4	101.325	(5.58) 4
		14.7	99.56	5.89
		20.2	137.5	7.70
		49.8	341.5	19.05
		62.7	430.4	22.44
		84.3	579.3	24.96
		100.5	691.0	25.98
100	310.9	$(0.949)^3$		
		(15.645) 4	101.325	(1.62) 4
		21.7	143.0	2.34
		33.7	225.7	3.88
100	310.9	52.5	355.3	6.23
				continued

¹Original data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A method is used in which water and propane are charged into an equilibration cell. After rocking for several hours, a sample of the aqueous solution is passed into an analysis train. The analysis consists of refluxing the water The analysis solution and collecting the evolved gas in an evacuated flask of known volume as well as pressure and temperature. This process is repeated until all the gas is removed. The quantity of water is determined by weight. Corrections are applied for the vapor pressure of water in the collection flask and for water collected in the cold trap connected to the gas collection flask.

SOURCE AND PURITY OF MATERIALS:

- 1. Phillips Petroleum Co. Certified purity of 99.9 mol per cent.
- 2. Distilled and deaerated.

ESTIMATED ERROR:

 $\delta P/P = 0.01$

 $\delta x_1/x_1 = 0.02$ (compiler)

²Calculated by compiler using vapor pressure data given by authors.

³Vapor pressure of water as given by authors.

[&]quot;Solubility for partial pressure of 101.325 kPa extrapolated by compiler.

INAL MEASUREMENTS: zarnoosh, A.; McKetta, J.J. et. Ref. 1958, 37, 275-278.		
et. Ref. 1958, 37, 275-278.		
PREPARED BY:		
. Hayduk		
ial Pressure ² Mol Fraction ¹ P_1/kPa 10^5x_1		
355.3 6.23 479.4 7.70 573.8 10.26		
660.0 10.50 784.1 12.44 797.9 12.56 822.0 13.62		
834.4 14.04 901.2 14.30 901.2 14.76 956.4 15.03		
959.8 15.41 977.1 15.67 039.1 16.87 097.7 16.91		
101.325 (0.99) 4 178.9 1.75 237.5 2.25		
246.5 347.8 3.48 383.3 4.02 523.6 5.20		
709.7 7.42 813.1 8.12 964.7 9.05		
123 10.65 254 12.10 .351 12.96 .571 14.17		
.637 15.06 .649 15.00 .654 15.07 .833 16.08		
17.30 1074 18.45 1343 20.00 1520 21.04		
26.22 21.50 101.325 (0.78) ⁴		
137.9 399.9 789.3 7.610 789.3 7.55		
1130 11.00 1230 11.69 1379 13.10 1665 15.12		
.768 16.80 .885 16.02		
continued		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propane; C ₃ H ₈ ; [74-98-6] (2) Water; H ₂ O; [7732-18-5]	Azarnoosh, A.; McKetta, J.J. Pet. Ref. 1958, 37, 275-278.
VARIABLES:	PREPARED BY:
T/K: 238.7-401.9 P/kPa: 99 - 3409	W. Hayduk

t 1/°F	T2/K	Total Pressure ¹ /psia	Partial Pressure ² P ₁ /kPa	Mol Fraction 1 /10 5x_1
220	377.6	305.7	1989	17.75
		310.7	2023	17.66
		314.0	2046	18.00
		355.7	2333	20.38
		408.7	2699	21.95
		425.7	2816	23.85
		447.2	3309	24.06
		497.2	3409	26.50
		511.7		27.00
280	410.9	(49.20) ³		
		(63.90) 4	101.325	(1.53) 4
		75.3	179.9	2.72
		125.4	525.2	6.04
		315.6	1836	19.65
		390.2	2350	23.60
		431.0	2632	27.24
		487.3	3020	29.20
		498.7	3098	31.30
				continued

¹Original data.

 $^{^{2}}$ Calculated by compiler using vapor pressure data given by authors.

 $^{^{\}rm 3}{\rm Vapor}$ pressure of water as given by authors.

 $^{^4 \}mbox{Solubility}$ for partial pressure of 101.325 kPa extrapolated by compiler.

COMPONENTS: (1) Propane; C₃H₈; [74-98-6] Azarnoosh, A.; McKetta, J.J. (2) Water; H₂O; [7732-18-5] Pet. Ref. 1958, 37, 275-278. VARIABLES: T/K: 288.7-410.9 P/kPa: 99-3409 PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

Smoothed data were presented by authors as follows:

Total Pressure ¹ /psia	T/K	Partial Pressure ² p ₁ /kPa	Mol Fraction 1 /10 5x_1	T/K	Partial Pressure ² p ₁ /kPa	Mol Fraction ¹ /10 ⁵ x ₁
	288.7	(1.765) ³		299.8	(3.50) ³	
14.7	(60°F)	99.6	5.7	(80°F)	97.9	2.45
20		136.1	7.5	• • • • •	134.4	3.38
40		274.0	14.95		272.3	6.65
60		411.9	22.15		410.2	10.05
80		549.8	24.50		548.1	13.40
100		687.7	25.9		686.0	16.60
108.5		746.3	(26.4) 4		-	-
146.0			-		1003	(21.9) 4
<u>-</u>	310.9	$(6.54)^3$		327.6	$(15.32)^3$	
14.7	(100°F)	94.8	1.52	(130°F)	86.0	1.08
20		131.4	2.15		122.6	1.55
40		269.2 407.1	4.51 6.85		260.5 398.4	3.18 4.84
60 80		545.0	9.20		536.3	6.45
100		682.9	11.51		674.1	8.09
150		1028	16.62		1019	12.09
191.5		1314	(20.3) 4			
200			-		1364	15.48
250		_	-		1708	18.54
275		-	-		1881	(20.0) 4
	344.3	(32.68) ³		360.9	$(64.40)^3$	
14.7	(160°F)	68.7	0.80	(190°F)	37.0	0.40
20		105.2	1.15		73.5	0.78
40		243.1	2.60		211.4	2.14
60 80		381.0	4.02 5.40		349.3 487.2	3.54 4.89
80 100		518.9 656.8	5.40 6.77		487.2 625.1	4.89 6.19
150		1002	10.03		969.8	9.29
200		1346	13.04		1315	12.12
250		1691	15.68		1659	14.83
300		2036	18.03		2004	17.31
350		2380	20.02		2349	19.58
389		2649	(21.2) 4		-	-
	360.9					
400		2693	21.37			
450		3038	22.98			
500		3383	24.20			
538	377.6	3645 (118.5) ³	(25.0) 4	394.3	$(205.7)^3$	
20	(220°F)		0.30	(250°F)	(203.7)	_
40	(220 F)	157.3	1.80	(230 1)	70.12	1.05
60		295.2	3.21		208.0	2.64
80		433.1	4.53		345.9	4.04
100		571.0	5.81		483.8	5.32
150		915.7	8.88		828.5	8.62
200		1260	11.99		1173	11.88

continued...

COMPONENTS: (1) Propane; C₃H₈; [74-98-6] Azarnoosh, A.; McKetta, J.J. (2) Water; H₂O; [7732-18-5] Pet. Ref. 1958, 37, 275-278. VARIABLES: T/K: 288.7-410.9 P/kPa: 99-3409 ORIGINAL MEASUREMENTS: Azarnoosh, A.; McKetta, J.J. Pet. Ref. 1958, 37, 275-278. W. Hayduk

EXPERIMENTAL VALUES: (concluded)

Total Pressure ¹ /psia	<i>T</i> /K	Partial Pressure ² p ₁ /kPa	Mol Fraction ¹ /10 ⁵ x ₁	T/K	Partial Pressure ² p ₁ /kPa	Mcl Fraction 1 /10 5x_1
250	377.6	1605	14.89	394.3	1518	15.19
300	(220°F)	1950	17.42	(250°F)	1863	17.94
350		2295	19.73	•	2207	20.58
400		2639	21.92		2552	22.90
450		2984	23.96		2897	24.38
500		3329	26.04		3242	28.72
	410.9	$(339.2)^3$				
60	(280°F)	74.46	1.19			
80		212.4	2.98			
100		350.3	4.51			
150		695.0	8.01			
200		1040	11.84			
250		1384	15.37			
300		1729	18.59			
350		2074	21.42			
400		2419	24.67			
450		2763	27.42			
500		3108	31.22			

¹Original smoothed values.

²Calculated by compiler based on vapor pressure data given by authors.

³Vapor pressures as given by authors but converted to kPa.

^{&#}x27;Incidence of two liquid phases.

- (1) Propane; C₃H₈; [74-98-6]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Wehe, A.H.; McKetta, J.J.

Anal. Chem. 1961, 33, 291-293.

VARIABLES:

T/K: 344.3 (160°F) P/kPa: 514.3-1247

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Gas Partial /psia¹	Pressure, P /kPa²	Mol Fraction ¹ 10 ⁵ ×1
74.6		
74.6 112.2	514.3 773.6	5.49 8.06
120.3	829.4	8.20
128.8	888.0	8.69
136.7	942.5	9.69
148.9	1027	10.1
165.0	1138	11.1
180.9	1247	12.3

¹Original data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water and propane were equilibrated in a cell at high pressure and constant temperature. A sample of the saturated aqueous solution was passed into a low pressure Orsat gas buret for gas release under controled conditions of temperature and pressure. At the low pressure used in the gas buret (usually < 200 mm mercury), Henry's law, and the ideal gas law, were assumed to describe the gas solubility, and volumetric properties, respectively. From a material balance and pressure-volume relationship, as well as the vapor pressure and volume of water in the gas buret, the hydrocarbon content of the original aqueous sample was calculated.

SOURCE AND PURITY OF MATERIALS:

- 1. Source and purity not given.
- 2. Treatment not specified.

ESTIMATED ERROR:

 $\delta P/P = 0.01$ (compiler) $\delta x_1/x_1 = 0.05$ (authors)

²Calculated by compiler.

- (1) Propane; C₃H₉; [74-98-6]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kobayashi, R.; Katz, D.L.

Ind. Eng. Chem. 1953, 45, 440-446.

VARIABLES:

T/K: 310.9-422.0

P/kPa: 490-3332

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t 1/°F	T/K	Total Pressure ¹ /psia	Partial Pressure ² P1/kPa	Mol Fraction /10 ⁵ x ₁
100	310.9	72	490	8.63
		117	800	15.52
133	329.3	188	1280	14.99
170	349.8	181	1207	11.46
		307	2075	17.63
190	360.9	131	839	7.96
		224	1480	13.30
		359	2411	19.60
205.7	369.7	230	1497	12.61
		400	2669	21.62
		478	3207	24.49
230	383.2	222	1387	13.01
		504	3332	26.33
260	399.8	170	928	10.01
		332	2045	19.64
		511	3279	28.92
300	422.0	265	1365	16.66
		471	2785	30.31

¹ Original data, excluding that involving a second liquid (propane) phase.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A high pressure cell containing propane and water was mechanically agitated for at least two hours to established equilibrium. Mercury was injected into the cell while the samples were taken. The analysis train consisted of a low pressure adsorption system for water vapor using magnesium perchlorate drying agent. The increase in gas pressure in a calibrated bottle was used to determine the amount of gas disolved. Real gas corrections were applied in determining the number of moles of propane.

Data were also given for the pressure at which a propane-rich liquid phase had just formed, defining the limit of the threephase system.

See next page.

SOURCE AND PURITY OF MATERIALS:

- Phillips Petroleum Co. Specified as 99 mol per cent minimum purity.
- 2. Distilled and degassed.

ESTIMATED ERROR:

T/K= 0.3

 $\delta P/P = 0.01$

 $\delta x_1/x_1 = 0.03$ (compiler)

²Calculated by compiler. Equilibrium data for three-phase systems also given in source.

(1) Propane; C₃H₈; [74-98-6]

(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kobayashi, R.; Katz, D. L.

Ind. Eng. Chem.

1953, 45, 440-446.

VARIABLES:

T/K: 278.9-369.5 P₁/MPa: 0.566-4.269 PREPARED BY:

W. Hayduk; C.L. Young

EXPERIMENTAL VALUES:

T/°F	T/K	Total Pressure P/psi	Partial Pressure p ₁ /MPa	Mole fraction of propane in liquid, ${}^x{\rm C}_3{\rm H}_6$
42.3	278.87	82.2	0.566	0.000366
53.9	285.32	101	0.695	0.0002913
78.1	298.76	142	0.976	0.0002208
79.1	299.31	143	0.979	0.0002208
100.2	311.04	191	1.310	0.0002045
100.6	311.26	191	1.310	0.0002001
132.9	329.21	284	1.941	0.0002046
137.7	331.87	300	2.050	0.0002003
154.2	341.04	366	2.495	0.0002063
160.3	344.42	391	2.663	0.0002107
172.2	351.04	446	3.032	0.0002298
179.7	355.21	482	3.272	0.0002360
189.6	360.71	538	3.645	0.0002495
191.1	361.54	543	3.678	0.0002489
201.7	367.43	608	4.109	0.0002638
205.4	369.48	632	4.269	0.0002726

Solubility given at pressure at which propane-rich liquid phase just forms, defining limit of three-phase region.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

High pressure cell with glass windows fitted with stirrer. System exhibits liquid-liquid-vapor equilibrium and cell fitted with sampling ports for the three phases. Liquid phase composition analysed by absorbing water on magnesium perchlorate and estimating gas volumetrically. Data on other phases in source.

SOURCE AND PURITY OF MATERIALS:

- Phillips Petroleum sample, purity 99 mole per cent or better.
- 2. Distilled and degassed.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.15$; $\delta P/MPa = \pm 0.01$ (up to 1.0 MPa); ± 0.05 (above 1.0 MPa); $\delta x_{C_3H_8} = \pm 10^{-6}$

(estimated by compilers)